

PHYS 643: Writing Hydro Codes

Eve J. Lee

Notes adapted from Prof. Andrew Cumming (McGill) and Dr. Paul Duffell (Harvard CfA).

1 Introduction

In general, fluid equations cannot be solved analytically, and instead need to be solved numerically. Here, we will cover the *basics* of how to write your own hydro solver. I'm only giving a very brief outline here. For more detailed discussions, you may consult the Heidelberg lectures (http://www.ita.uni-heidelberg.de/~dullemond/lectures/num_fluid_2011/)

2 First Order Finite Differencing

The whole idea behind this method is to define some fluid quantity as a function of time and space over some discrete spatial grid. Consider 1-dimensional advection-diffusion equation of some variable f :

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = D \frac{\partial^2 f}{\partial x^2} \quad (1)$$

where D is some constant diffusivity and velocity u is assumed constant. This should look a lot like Navier-Stokes equation for incompressible flows in the absence of gravity and pressure gradient forces.

We will calculate the quantity f on a 1-dimensional grid such that f_j is the value of f at $x = x_j$ where $j = 1$ to N (N is an integer). For simplicity, we will consider uniform grid spacing: $x_{j+1} - x_j = \Delta_x$.¹ In order to solve the advection-diffusion equation, we need to define the derivative of f , $f'_j \equiv \partial_x f$ at $x = x_j$, and $f''_j \equiv \partial_x^2 f$ at $x = x_j$. From Taylor expansion:

$$f_{j+1} = f_j + \Delta_x f'_j + \frac{\Delta_x^2}{2} f''_j + O(\Delta_x^3) \quad (2)$$

$$f_{j-1} = f_j - \Delta_x f'_j + \frac{\Delta_x^2}{2} f''_j - O(\Delta_x^3) \quad (3)$$

We can subtract these two to obtain an expression for f'_j :

$$f'_j = \frac{f_{j+1} - f_{j-1}}{2\Delta_x} + O(\Delta_x^2). \quad (4)$$

Notice how the error is on the order of Δ_x^2 ; this expression is accurate to second order.

By adding equations 2 and 3, we can define f''_j :

$$f''_j = \frac{f_{j+1} - 2f_j + f_{j-1}}{\Delta_x^2} + O(\Delta_x^2). \quad (5)$$

We have all the required expressions to define the time evolution of the quantity f ! Let us first consider just the advection:

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 0 \quad (6)$$

We will label f at different time with superscript n so that the above advection equation can be written as:

$$\frac{f_j^{n+1} - f_j^n}{\Delta_t} = -u \frac{f_{j+1}^n - f_{j-1}^n}{2\Delta_x}, \quad (7)$$

¹In real-life research application, we often use variable grid spacing that is based on the resolution requirement (“adaptive mesh refinement”) or based on some sort of tessellation scheme.

so that I can update the value of f_j in time according to

$$f_j^{n+1} = f_j^n - \frac{u\Delta_t}{2\Delta_x}(f_{j+1}^n - f_{j-1}^n). \quad (8)$$

Since f^{n+1} is defined only in terms of f^n , this is called “explicit” method. In fact, this particular definition is called Forward-Time Central-Space (FTCS) method. If you try to solve the advection equation using the FTCS method, you will find that your numerical solution is unstable!

2.1 Von Neumann Stability Analysis

How can we assess a priori whether the chosen numerical method will be stable vs. unstable? In general, a solution can be expressed as a finite Fourier series with amplitude ξ^n that depends on time. Let’s consider just one component:

$$f_j^n = \xi^n e^{ik(j\Delta_x)}. \quad (9)$$

For the solution to be stable, we need to ensure $|\xi^{n+1}/\xi^n| < 1$ for all wavenumber k ; otherwise, f will grow exponentially with time. Let’s substitute equation 9 into equation 8 to assess the stability of FTCS scheme:

$$\begin{aligned} e^{ik(j\Delta_x)}\xi^{n+1} &= e^{ik(j\Delta_x)}\xi^n - \frac{u\Delta_t}{2\Delta_x}(\xi^n e^{ik(j+1)\Delta_x} - \xi^n e^{ik(j-1)\Delta_x}) \\ \frac{\xi^{n+1}}{\xi^n} &= 1 - \frac{u\Delta_t}{2\Delta_x}(e^{ik\Delta_x} - e^{-ik\Delta_x}) \\ &= 1 - \frac{u\Delta_t}{\Delta_x}i \sin k\Delta_x \\ \left| \frac{\xi^{n+1}}{\xi^n} \right| &= \left| 1 + \left(\frac{u\Delta_t}{\Delta_x} \right)^2 \sin^2(k\Delta_x) \right|, \end{aligned} \quad (10)$$

which is always larger than 1 so FTCS scheme is unstable.

2.2 Lax-Friedrichs method

We replace equation 8 with

$$f_j^{n+1} = \frac{1}{2}(f_{j+1}^n + f_{j-1}^n) - \frac{u\Delta_t}{2\Delta_x}(f_{j+1}^n - f_{j-1}^n). \quad (11)$$

From stability analysis,

$$\begin{aligned} \left| \frac{\xi^{n+1}}{\xi^n} \right| &= \left| \cos^2(k\Delta_x) + \left(\frac{u\Delta_t}{\Delta_x} \right)^2 \sin^2(k\Delta_x) \right| \\ &= \left| 1 + \sin^2(k\Delta_x) \left[\left(\frac{u\Delta_t}{\Delta_x} \right)^2 - 1 \right] \right|. \end{aligned} \quad (12)$$

The Lax-Friedrichs method is stable if

$$\Delta_t \leq \Delta_x/u, \quad (13)$$

i.e., the timestep of integration needs to be shorter than the advection time across a grid cell. This is called the “Courant” condition.

Note that computational error emerges as “numerical viscosity”. Equation 11 can be re-written as

$$\frac{f_j^{n+1} - f_j^n}{\Delta_t} = -u \left(\frac{f_{j+1}^n - f_{j-1}^n}{2\Delta_x} \right) + \frac{1}{2} \left(\frac{f_{j+1}^n - 2f_j^n + f_{j-1}^n}{\Delta_x^2} \right), \quad (14)$$

which is the FTCS representation of

$$\frac{\partial f}{\partial t} = -u \frac{\partial f}{\partial x} + \frac{\Delta_x^2}{2\Delta_t} \frac{\partial^2 f}{\partial x^2} \quad (15)$$

where the last term represents numerical viscosity.

2.3 Godunov method (Upwind differencing)

Note that in Lax-Friedrichs method, the information of both the $(j+1)$ 'th and the j 'th cells propagate to the j 'th cell which is unphysical given that the advection velocity u has one direction. To avoid this, we further make the following adjustment:

$$f_j^{n+1} = \begin{cases} f_j^n - u_j^n \frac{\Delta t}{\Delta x} (f_j^n - f_{j-1}^n) & \text{if } u_j^n > 0 \\ f_j^n - u_j^n \frac{\Delta t}{\Delta x} (f_{j+1}^n - f_j^n) & \text{if } u_j^n < 0 \end{cases} \quad (16)$$

where u_j^n is the advection velocity at grid j at time n . The same Courant condition as before needs to be satisfied for stability.

2.4 Taking Care of Diffusion

Isolating the diffusion term:

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}. \quad (17)$$

We could use finite differencing but the computation time scales quadratically with the grid size. Instead, use an implicit scheme:

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = \frac{D}{(\Delta x)^2} (f_{j+1}^{n+1} - 2f_j^{n+1} + f_{j-1}^{n+1}) \quad (18)$$

which can be re-written as

$$-\beta f_{j+1}^{n+1} + (1 + 2\beta) f_j^{n+1} - \beta f_{j-1}^{n+1} = f_j^n \quad (19)$$

with $\beta = D\Delta t/(\Delta x)^2$. This can be further re-written as $A\vec{f}^{n+1} = \vec{f}^n$ with A a tri-diagonal matrix with elements $-\beta$, $(1 + 2\beta)$, and $-\beta$ so that \vec{f}^{n+1} can be solved by inverting A : $\vec{f}^{n+1} = A^{-1}\vec{f}^n$.

2.5 Operator Splitting

Now that we know how to solve advection and diffusion equations separately, how do we solve the advection-diffusion equation? Simply add them by means of splitting the operator.

2.5.1 Explicit method

First update your grid with the diffusion term:

$$f_j^{n+1} = f_j^n + \beta(f_{j+1}^n - 2f_j^n + f_{j-1}^n), \quad (20)$$

then calculate the advection term:

$$f_j^{n+1} = \frac{1}{2}(f_{j+1}^n + f_{j-1}^n) - \alpha(f_{j+1}^n - f_{j-1}^n) \quad (21)$$

with $\alpha = u\Delta t/\Delta x$.

Here's a Python code snippet with `T` some array with `n` elements:

```
T[1:n-1] += beta * (T[:n-2] + T[2:] - 2.0 * T[1:n-1]) #diffusion
T[1:n-1] = 0.5 * (T[:n-2] + T[2:]) - 0.5 * alpha * (-T[:n-2] + T[2:]) #advection
```

2.5.2 Implicit method

As before, first update your grid with the diffusion term but using the implicit scheme. Here's a Python code snippet on calculating the diffusion term:

```
import numpy as np
```

```
A = np.eye(n) * (1.0 + 2.0 * beta) + np.eye(n, k=1) * -beta + np.eye(n, k=-1)*-beta
#Apply appropriate boundary conditions on A
T = np.linalg.solve(A, T)
```

Advection terms can be calculated afterward as before.

2.5.3 Boundary conditions on the matrix A

There are two different boundary conditions on the fluid velocity when it comes to diffusive motion: no-slip (zero relative velocity with respect to the hard boundary) and stress-free (zero velocity gradient). Let's consider the hard surface to be situated at the left boundary of the grid and impose stress-free condition at the right boundary of the grid. You should have the initial condition on the fluid velocity such that $v[0]$ is set to the speed of the boundary. Then, you need to ensure $v[0]$ stays fixed at all times:

$$\begin{aligned} A[0][0] &= 1 \\ A[0][1] &= 0 \end{aligned}$$

This ensures the first element is fixed and that there is no diffusive flux through the first element.

What about the stress-free condition at the right boundary? You want to make sure that the $f_{j+1} - f_j$ term and the $f_j - f_{j-1}$ term goes to zero at the right-most boundary in equation 19. This can be done by $A[-1][-1] = 1 + \text{beta}$

3 Finite Volume Methods

Recall that fluid equations are nothing more than statements of conservation (conservation of mass, conservation of momentum, conservation of energy), and follow the form

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}(uf) = (\text{sources and sinks}) \quad (22)$$

(i.e., the rate of change of f + the flux of f is controlled by the sources and sinks of f).

In this method, we divide the volume into cells and we track the rate of change of f in the j -th cell by calculating the net flux of f through the cell:

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = \frac{J_{j-1/2} - J_{j+1/2}}{\Delta x} \quad (23)$$

where the cell location is x_j and its boundaries are $x_{j-1/2}$ and $x_{j+1/2}$. We need to define the flux J .

3.1 Donor Cell Advection: Hydro code example

Letting $f_1 = \rho$ and $f_2 = \rho u$, with $P = \rho c_s^2 = f_1 c_s^2$ and c_s being constant, the continuity and the Euler equation (in the absence of body force) can be written as

$$\begin{aligned} \frac{\partial f_1}{\partial t} + \frac{\partial}{\partial x}(uf_1) &= 0 \\ \frac{\partial f_2}{\partial t} + \frac{\partial}{\partial x}(uf_2) &= -\frac{\partial P}{\partial x}. \end{aligned} \quad (24)$$

3.1.1 First consider no source term

From continuity equation, we can update

$$f_{1,j}^{n+1/2} = f_{1,j}^n - \frac{\Delta t}{\Delta x}(J_{1,j+1/2} - J_{1,j-1/2}) \quad (25)$$

In donor cell advection scheme, we assume f_1 and f_2 are constant within the cell so that

$$J_{1,j+1/2} = \begin{cases} u_{j+1/2}^n f_{1,j}^n, & u_{j+1/2}^n > 0 \\ u_{j+1/2}^n f_{1,j+1}^n, & u_{j+1/2}^n < 0 \end{cases}$$

and

$$J_{1,j-1/2} = \begin{cases} u_{j-1/2}^n f_{1,j-1}^n, & u_{j-1/2}^n > 0 \\ u_{j-1/2}^n f_{1,j}^n, & u_{j-1/2}^n < 0 \end{cases}$$

where the velocity at the cell interface is defined as

$$u_{j+1/2}^n = \frac{1}{2} \left(\frac{f_{2,j}}{f_{1,j}} + \frac{f_{2,j+1}}{f_{1,j+1}} \right). \quad (26)$$

We follow the same scheme for f_2 with $\partial P / \partial x = 0$.

3.1.2 Add the source term

No explicit source term for continuity so mass is simply conserved:

$$f_{1,j}^{n+1} = f_{1,j}^{n+1/2}. \quad (27)$$

For the Euler equation, we need to consider the pressure gradient:

$$f_{2,j}^{n+1} = f_{2,j}^{n+1/2} - \frac{\Delta_t}{\Delta_x} c_s^2 (f_{1,j+1}^{n+1/2} - f_{1,j-1}^{n+1/2}) \quad (28)$$

3.1.3 Boundary conditions

There are many different kinds of boundary conditions. The most common ones are: fixed boundaries, outflow (flows past the simulation boundary are lost forever), periodic (i.e., loops back to other side), or reflective. We'll only consider reflective boundaries here. Simply apply:

$$\begin{aligned} f1[0] &= f1[0] - (dt / dx) * J1[0] \\ f1[-1] &= f1[-1] + (dt / dx) * J1[-2] \end{aligned}$$

and likewise for f_2 and J_2 to “reflect” the advection term. For the computational implementation for donor cell advection, refer to http://www.ita.uni-heidelberg.de/~dullemond/lectures/num_fluid_2011/Chapter_5.pdf.